Electron-phonon interaction and antiferromagnetic correlations

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We study effects of the Coulomb repulsion on the electron-phonon interaction (EPI) in a model of cuprates at zero and finite doping. We find that antiferromagnetic correlations strongly enhance EPI effects on the electron Green's function with respect to the paramagnetic correlated system, but the net effect of the Coulomb interaction is a moderate suppression of the EPI. Doping leads to additional suppression, due to reduced antiferromagnetic correlations. In contrast, the Coulomb interaction strongly suppresses EPI effects on phonons, but the suppression weakens with doping.

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There are strong experimental indications that the electron-phonon interaction (EPI) plays a substantial role for properties of high-T_c cuprates [1, 2], and that it even can lead to formation of small polarons for undoped cuprates [3]. The Coulomb interaction in the copper-oxide plane is expected to strongly suppress charge fluctuations. This is often described in the Hubbard or t-J [4] models, for which important phonons couple to such charge fluctuations [5]. One might therefore actually expect the Coulomb interaction to strongly suppress the EPI. This was indeed found with dynamical mean-field theory [6, 7] calculations in the paramagnetic phase (P-DMFT) [8, 9, 10]. On the other hand, calculations for the undoped antiferromagnetic t-J model using the self-consistent Born approximation (SCBA) [11], or approximations going beyond the SCBA [12], found that the Coulomb interaction enhances EPI effects on the electron Green's function.

The half-filled Hubbard model becomes an insulator for large U. In the P-DMFT the only mechanism for this is the quasiparticle weight Z going to zero [7]. Such a reduction of Z tends to strongly suppress the EPI [10, 11], which is an important reason for the small effects of the EPI in the P-DMFT. By allowing for antiferromagnetism (AF) in the DMFT [13, 14, 15], it is possible to have an insulating state although Z remains finite. This suggests that it is important to allow for AF when describing the EPI, i.e., using an AF-DMFT. This is also suggested by the fact that in the SCBA, the enhancement of the EPI grows with the value of the exchange constant J [11], i.e., with the importance of the AF.

Here we therefore use an AF-DMFT formalism and we first consider a half-filled system. In contrast to previous work, we find that within the Holstein-Hubbard model the effects of the EPI on the electron Green's function are neither strongly suppressed nor enhanced by the Coulomb interaction. While previous work could only address [11, 12] the half-filled case, the present formalism makes it possible to treat doped metallic cuprates, which are of particular interest. We show that the EPI remains important for the electron Green's function as long as AF is important. Due to the weakening of AF correlations as the system is doped, we find that doping reduces the effects of the EPI on the electron Green's function and it weakens the tendency to polaron formation, in agreement with experimental results [3].

We also calculate the renormalization of the phonon frequency. For the undoped system, we find that the Coulomb repulsion very strongly suppresses the renormalization. As the system is doped, however, the renormalization of the phonon frequency increases. This is the opposite behavior to what we find for the electron Green's function. The width and softening of the phonon spectral function is often used to estimate the strength of the EPI [16]. These results show that for strongly correlated systems this approach may strongly underestimate the EPI [17, 18].

We study the Holstein-Hubbard model

$$H = -t \sum_{\langle ij\rangle\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$
$$+ \ \omega_0 \sum_i b_i^\dagger b_i + g \sum_i (n_i - 1)(b_i + b_i^\dagger),$$

where $c_{i\sigma}^\dagger$ creates an electron with spin σ on site i and b_i a phonon on site i, $t > 0$ is a hopping integral, U the Coulomb interaction between two electrons on the same site, ω_0 is the phonon energy, g a coupling constant and n_i measures the number of electrons on site i. We assume an infinite-coordination Bethe lattice with the half band width D and the density of states (DOS) $N(\varepsilon) = (2/\pi D^2)\sqrt{D^2 - \varepsilon^2}$. We define a dimensionless coupling constant $\lambda = g^2/(\omega_0 D)$. For large U the Hubbard model is approximately equivalent to the t-J model. For a two-dimensional (2d) lattice, these models are related via $J/t = D/U$.

We solve the DMFT equations for the temperature $T = 0$. The associated impurity problem is solved using the Lanczos method. The Hilbert space is limited by only allowing up to N_{ph} phonons, where $N_{ph} \sim 30$ depends on the parameters. The energies of and couplings to the bath levels are determined from a continued fraction expansion [19] for the large U half-filled case and otherwise by a fit of the cavity Green's function on the imaginary axis [20]. We use up to 25 bath levels.

We here focus on the quasi-particle weight Z, since our criterion for polaron formation is Z being exponentially small and since Z_0, calculated for $\lambda = 0$, is expected to be crucial for the EPI, as discussed above. Fig. 1 shows Z_0 as a function of U for the half-filled Hubbard model according to AF-DMFT and P-DMFT and as a function of J for the (2d) t-J model according to the SCBA. The SCBA results agree well with exact diagonalization results for small clusters [21]. The half-filled system is an insulator in the AF-DMFT and for $U \gtrsim 3D$ in the P-DMFT [15]. While Z_0 drops to zero very quickly with U in the P-DMFT, it remains finite in the AF-DMFT. For U/D values where the Hubbard and t-J models are approximately equivalent, AF-DMFT and SCBA agree rather well. This good description of Z_0 suggests that AF-DMFT may describe the EPI well.
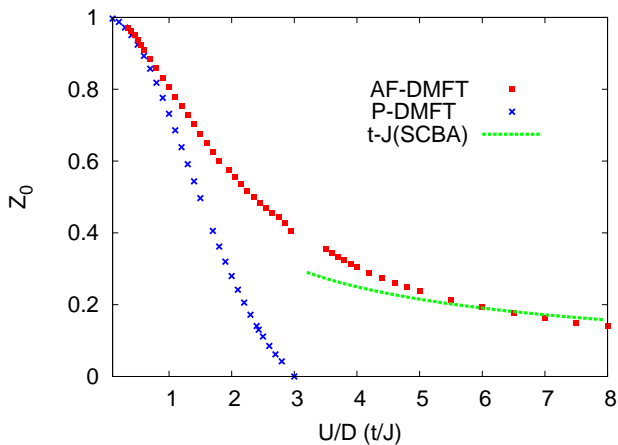

FIG. 1: Quasiparticle weight Z_0 for $\lambda = 0$ for the Hubbard model (as a function of U/D) according to P-DMFT and AF-DMFT and for the 2d t-J model (as a function of J/t) according to the SCBA. The figure illustrates that the AF-DMFT gives reasonable values for Z_0.

We first discuss the results for a weak EPI. For noninteracting electrons ($U = 0$), the reduction of Z by the EPI is given by $(1/Z - 1)/\lambda = 4/\pi$ for small λ and $\omega_0 \ll D$, as shown by the arrow in Fig. 2. To determine the effect of the EPI for interacting electrons ($U > 0$), we calculate $(Z_0/Z - 1)/\lambda$, shown in Fig. 2. This quantity measures how efficiently the EPI reduces the quasiparticle weight Z with respect to Z_0 obtained in the absence of EPI. In a P-DMFT calculation it was found that the

EPI very quickly becomes inefficient when U is increased [10]. In contrast, allowing for AF, we find that the EPI remains much stronger as U is increased, although it is still reduced compared to the noninteracting case. These results show that AF is crucial for the EPI of the half-filled system. For U/D values where the Hubbard and t-J models can be compared, the AF-DMFT and the SCBA agree well for $\omega_0 = 0.025D$. For larger phonon frequencies, however, we find that the EPI is appreciably more efficient in the SCBA than in the AF-DMFT.
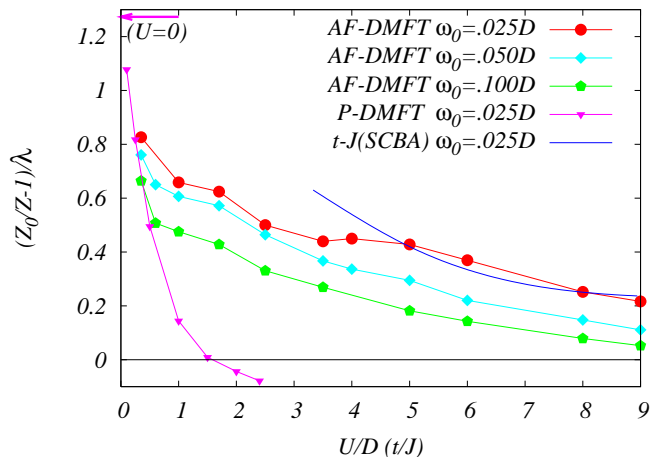

FIG. 2: $(Z_0/Z - 1)/\lambda$ in the limit $\lambda \to 0$ for the Hubbard model according to the P-DMFT and AF-DMFT and for the t-J model according to the SCBA. This quantity indicates the effectiveness of the EPI in the weak-coupling limit. The figure illustrates how the EPI is much more efficient in the AF-DMFT than the P-DMFT, and that AF-DMFT and SCBA agree rather well.

We next focus on strong EPI. Fig. 3 shows Z as a function of λ for different U. The result for $U = 3.5D$ ($J/t = 0.29$) can be compared with a calculation for the 2d t-J model [12] ($J/t = 0.3$ and the same ω_0). As λ is increased, Z is strongly reduced, signaling polaron formation. This happens at a somewhat larger critical value λ_c than was found for the t-J model [12], indicated by an arrow. The deviation from Ref. [12] is probably mainly due to our use of the AF-DMFT and the neglect of "crossing" diagrams in Ref. [12]. Good agreement is also found with results for the infinite dimension t-J model [22]. These comparisons suggest that the AF-DMFT is rather accurate for the half-filled Holstein-Hubbard model.

For $U = 0$, Z drops very quickly as a function of λ and (bi-)polarons are formed at $\lambda_c \approx 0.33$. As U is increased the drop is slightly less rapid and polaron formation happens at somewhat larger λ_c. The Coulomb interaction therefore moderately suppresses polaron formation.

In P-DMFT calculations it was found that the effective mass m^* depends only weakly on ω_0 [10]. In AF-DMFT we find a sizable isotope effect on m^* and for $\lambda \sim \lambda_c$ the
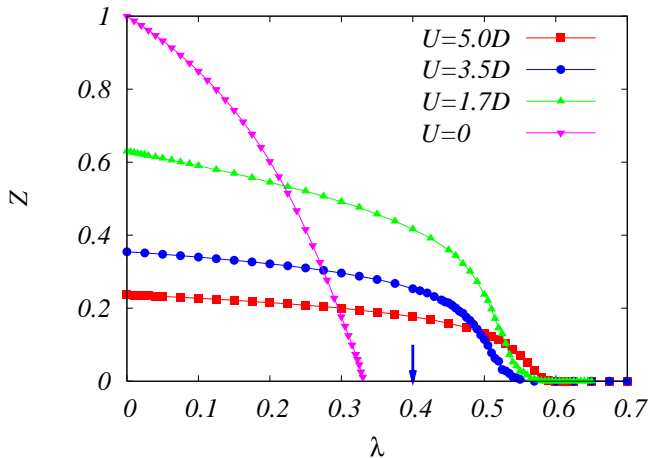
FIG. 3: Z as a function of λ for different U and for $\omega_0 = 0.025D$. The arrow shows λ_c of the t-J model for $J/t = 0.3$ ($U/D = 3.3$) [12]. The figure shows how the Coulomb interaction moderately suppresses polaron formation ($Z \to 0$).

FIG. 4: Z as a function of λ for different fillings n and associated magnetic moments m for $U = 3.5D$ and $\omega_0 = 0.025D$. The figure illustrates how the critical λ_c is increased as the filling is reduced (doping is increased) due to a reduction of the the antiferromagnetic correlations.

effect is comparable to the experimental value [23].

Above we have discussed the half-filled system extensively, since we can compare with other methods and test the reliability of the AF-DMFT. The doped cuprates, however, are more interesting and challenging, and we now focus on them. Fig. 4 shows Z as a function of λ for $U = 3.5D$ and for different dopings. As the filling is reduced (hole doping increased) the staggered magnetization m is reduced. The figure shows how this leads to an increase in λ_c. In a P-DMFT calculation [10], on the other hand, a reduction of the filling leads to a reduction of λ_c. The increase of λ_c in the AF-DMFT with increased doping is therefore indeed due to the reduction of m, since at constant $m = 0$, λ_c decreases with doping.

We find the AF-P transition for $U = 3.5D$ at $n = 0.84$, corresponding to a much larger doping (0.16) than found experimentally. This is only partly due to our neglect of second nearest neighbor hopping which would introduce magnetic frustration in the system. The main reason is that in the P state there are also AF correlations which lower the energy, but which are neglected in a DMFT calculation. The AF-DMFT calculation therefore favors the AF state. To obtained a balanced treatment it is necessary to use a cluster DMFT method [24, 25]. Such a calculation would introduce AF correlations also in the P state, and like in the AF-DMFT calculation these correlations would weaken as the doping is increased. This should increase λ_c with doping in a qualitative similar way as in Fig. 4.

Experimentally, polaron formation is found to disappear as the system is moderately doped [3]. This may be partly due to screening of the EPI, leading to a reduction of λ. However, the suppression of polaron formation with
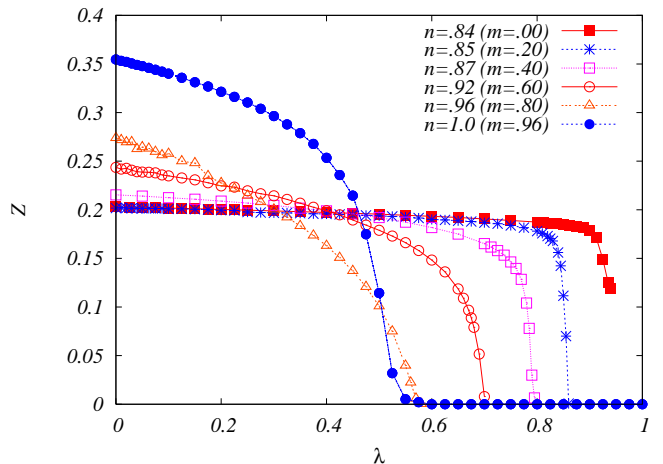
doping for fixed λ, illustrated in Fig. 4, should also be an essential part of the explanation.

To study effects of the Coulomb interaction, earlier work compared with a Holstein model with a single electron at the bottom of the band [11, 12]. A better comparison, however, is with a half-filled Holstein model, since we can then increase U keeping the number of electrons unchanged. For a half-filled 2d Holstein model such a comparison is difficult, due to Fermi surface nesting and phase transitions. In DMFT calculations using a Bethe lattice this is not a problem.

The EPI appears much stronger for the half-filled Holstein model than for a single electron at the bottom of the band. Comparing with the half-filled case, we therefore find that the EPI is suppressed by the Coulomb interaction, while earlier studies, comparing with the single electron case, found an enhancement.

To discuss the difference between the two cases for a weak EPI, we calculate the electron-phonon part of the electron self-energy (g and ω small, $\omega_0 \ll D$)

$$\mathrm{Re}\Sigma_{\mathrm{ep}}(\omega) = -\alpha \frac{2g^2}{8\pi\omega_0 t}\omega, \qquad (2)$$

where $\alpha = 1$ for the 2d single electron case but $\alpha = 4$ for the half-filled case with a semi-elliptical DOS. This large difference is partly due to the DOS of the 2d Holstein model being smallest at the bottom of the band, and partly due to Re Σ_{ep} having contributions both from higher and lower states for the half-filled case, but only from higher states for the single electron case.

To understand the difference for a strong EPI, we study polaron formation in the adiabatic limit by comparing states with free electrons and perfectly localized electrons

[26]. We find $E_{\text{free}} = -4\beta t$ per electron, where $\beta = 1$ (one electron) or $\beta = 4/(3\pi) \approx 0.42$ (half-filled case), and $E_{\text{loc}} = -g^2/\omega_{\text{ph}}$ per electron for both cases. We assume that polarons form when $|E_{\text{loc}}| > |E_{\text{free}}|$. This leads to a large $\lambda_c = 1$ [27] for a single electron and a much smaller $\lambda_c = 0.42$ for the half-filled case [29].

We emphasize the remarkably small value, $\lambda_c = 0.33$, for polaron formation in a half-filled Holstein model, meaning that Migdal's theorem breaks down for quite small λ. Using different values for ω_0, small λ_c have also been obtained earlier [30, 31, 32, 33] using DMFT calculations.
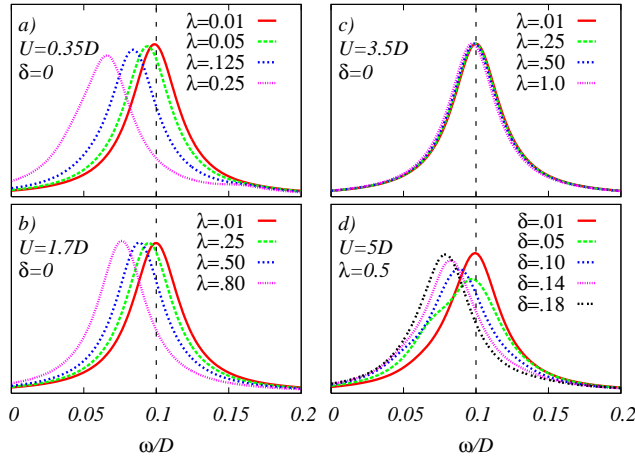

FIG. 5: Phonon spectral function for different values of λ. The bare phonon frequency is $\omega_0 = 0.1D$ and a Lorentzian broadening with the full width half maximum of 0.04 D has been introduced. The figures a-c show how the phonon softening at half-filling is dramatically suppressed by U and figure d that the softening increase with doping δ.

We now consider the influence of the EPI on phonons. Fig. 5a shows the phonon spectral function for a small U at half-filling (doping $\delta = 0$) for different EPI strengths. The figure illustrates how the phonon is softened substantially as the EPI is increased. Fig. 5b-c show this softening is strongly reduced when U is increased. The reason is that for large U charge fluctuations are strongly suppressed, and the system can only respond weakly to a phonon which couples to the net charge on the atoms. Fig. 5d shows how the softening increases as the doping is increased, due to the doped holes responding to phonons. This is in agreement with neutron scattering measurements [2]. The figure illustrates that the influence of the EPI on the phonon self-energy is dramatically different from the influence on the electron self-energy. The reason is that the electron self-energy measures the response of the system to the removal or addition of a charge, which leads to a strong response even in cases where charge fluctuations are otherwise suppressed.

While paramagnetic DMFT calculations for the Holstein-Hubbard model show that effects of the EPI on *electrons* (quasiparticle weight) are very strongly suppressed by the Coulomb interaction, we find that this suppression is only moderate when antiferromagnetic (AF) correlations are included. As the doping is increased, the AF is reduced and the EPI is more suppressed. In contrast, at half-filling, the Coulomb interaction strongly suppresses effects of the EPI on *phonons* (phonon softening), while the suppression is reduced with doping. These trends are consistent with experiment.

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